

1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-
376-18-1 | DTXSID3059923

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 54.2 °C

Global applicability domain: Outside

Local applicability domain index: 4.02e-01

Confidence level: 6.20e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9- hexadecafluoro- Measured: 56.0 Predicted: 54.2</div>	<div>Image not found</div> <div>PFOA Measured: 55.0 Predicted: 53.2</div>	<div>Image not found</div> <div>Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7- dodecafluoro- Measured: 34.0 Predicted: 32.9</div>
<div>Image not found</div> <div>Heptafluorobutyric acid Measured: -17.5 Predicted: -14.1</div>	<div>Image not found</div> <div>Perfluorododecanoic acid Measured: 108 Predicted: 103</div>	